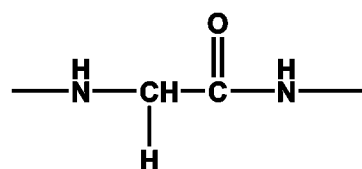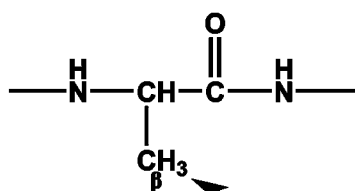Figure 1. Convention for designating positions along amino acid residue side-chain. This convention is used regardless of atom type and branching.
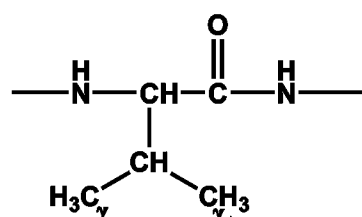
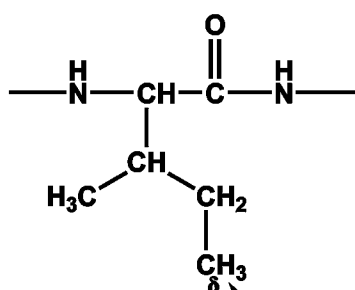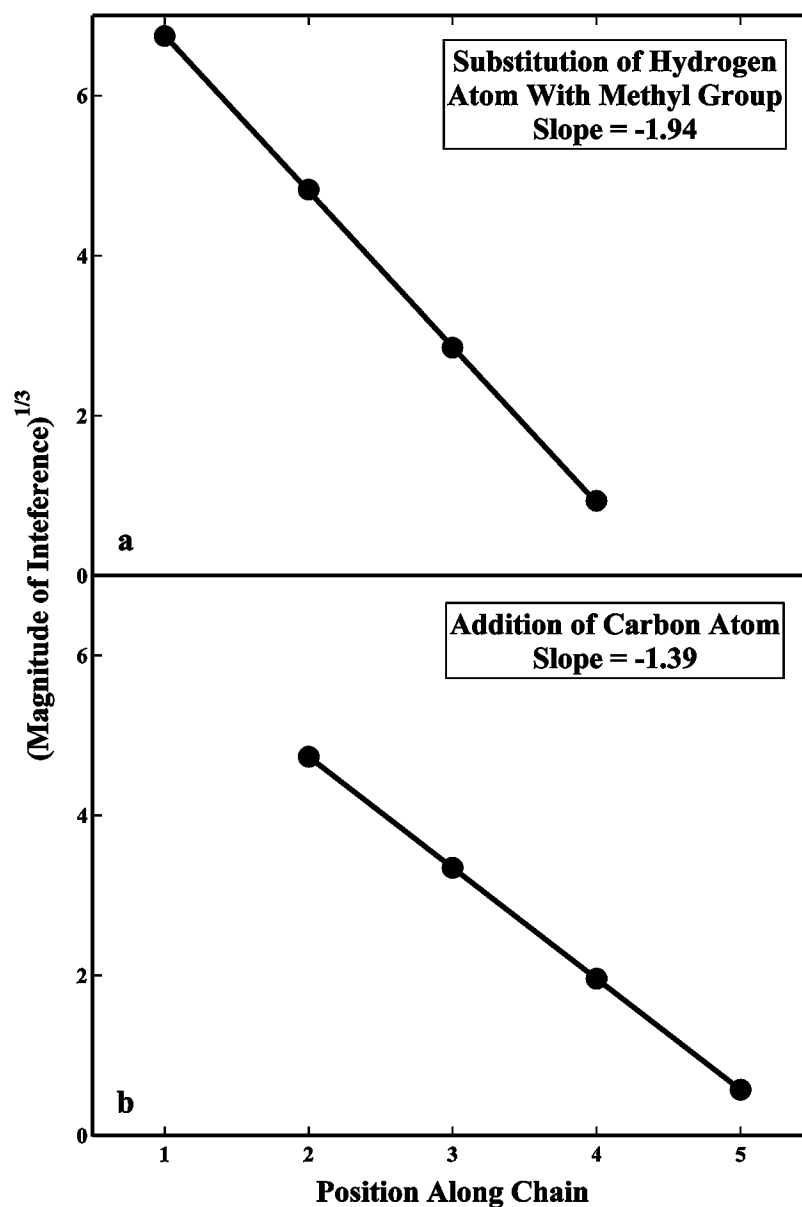Figure 2. Outline of method for calculating coefficients.

Figure 3.   Graph of the cube roots of the methyl substitution for hydrogen coefficients (a) and carbon atom coefficients alone (b) as a function of the position along the carboxyl residue side chain. The β, γ, and δ points for (a) were calculated directly from the experimental data. The ε point is dependent on the individual atom calculations. The linearity of (b) was used to optimize the individual atom coefficients. As expected in this theoretical treatment, the fractional volume occupied by a linear side chain decreases with the cube root of the substituent number.
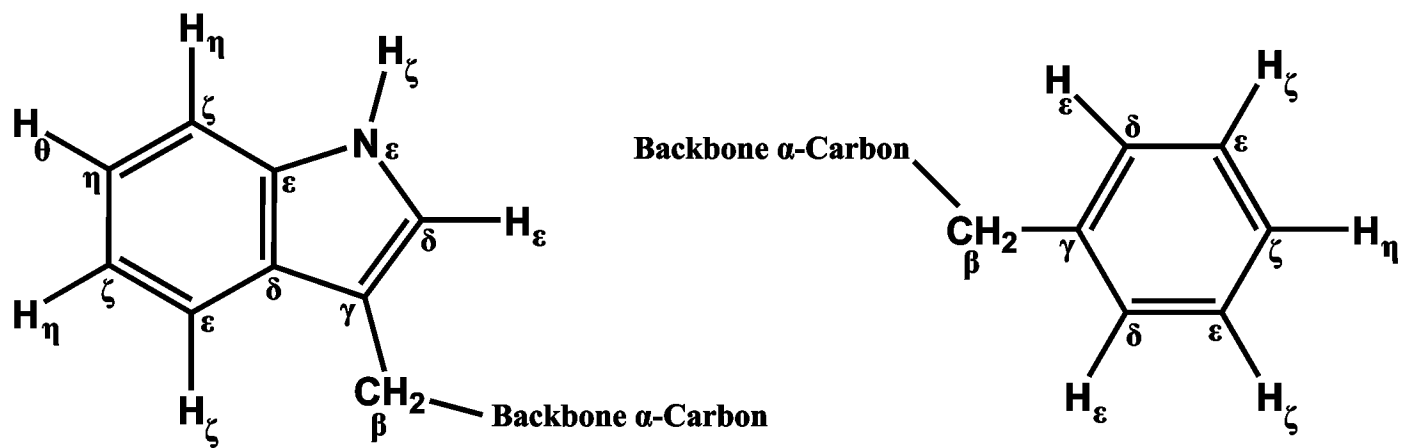
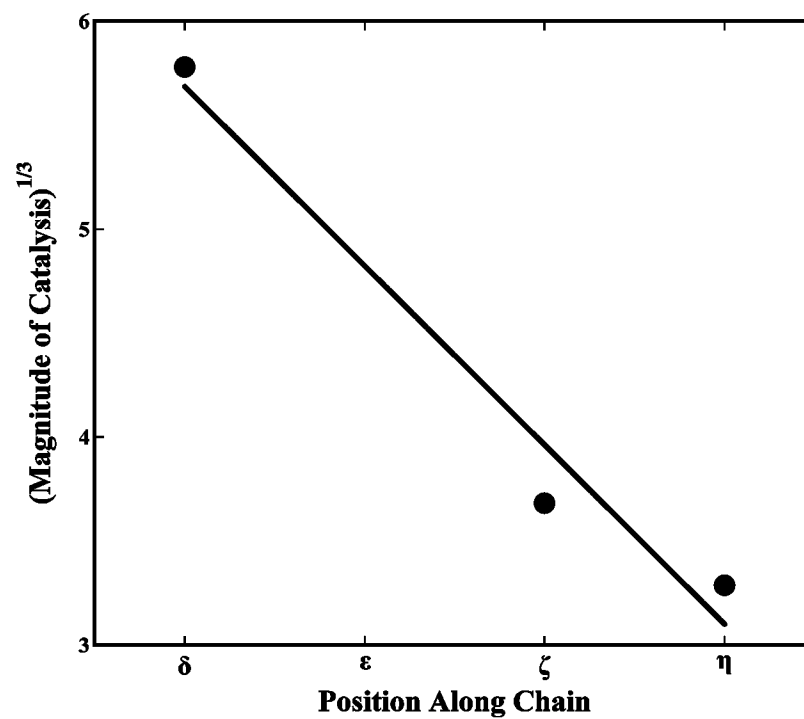Figure 4. Convention for labeling positions on the Trp and Phe sidechains.

Figure 5. Graph of the cube root of the NH+ catalysis coefficients for His, Lys, and Arg as a function of position along the carboxyl-side residue side chain.
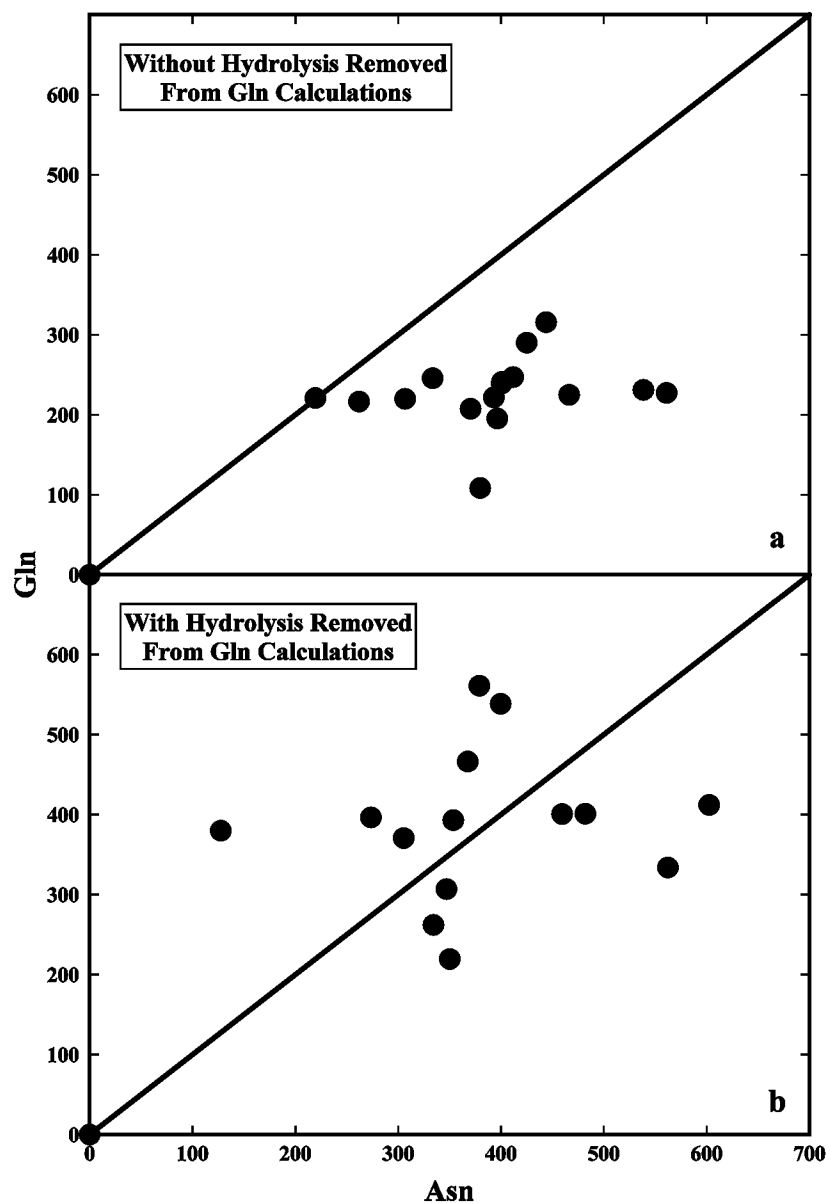
Figure 6.   (a) Normalized Gln (100)(ln(k)) without hydrolysis corrections vs. those for Asn (100)(ln(k)) with hydrolysis corrections as listed in Table 1. The fundamental difference in succinimide rate vs. glutarimide rate has been removed by normalization, which subtracts the Gln values from GlyXxxGlnGlyGly and the Asn values from GlyXxxAsnGlyGly. (b) As in (a) with both the Asn and Gln values corrected for hydrolysis. The two dimensional medians of the plotted points are indicated by the squares.